Development and Current Status of Korea Thermophysical Properties Databank (KDB) [1]

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[1] Paper presented at the Fourteenth Symposium on Thermophysical Properties, Jun 25-30, 2000, Boulder, Colorado, U.S.A.

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ABSTRACT

Physical property data, equilibrium data and prediction models are essential part of process design and operation. With the financial support of Ministry of Commerce, Industry and Energy (MOCIE) of Korea, four universities collaborated to construct thermophysical databank and experimental data production. In this paper topics relating to the construction and use of thermophysical properties and equilibrium database are discussed. The databank contains about 4000 pure compounds and 5000 equilibrium data sets. Most of the data were collected along with their accuracy of measurements or experimental uncertainties. Various estimation methods and thermodynamic models were included to calculate properties and phase equilibria. Data can be searched by stand-alone program or Internet WEB site. The current status and prospect of KDB (Korean thermophysical properties DataBank) are discussed.

KEYWORDS : database; data bank; data collection; physical property ; thermophysical property; vapor-liquid equilibrium

1.Introduction

Physical properties and equilibrium data are raw material for the process design and operations. Thermophysical and equilibrium property data for components and mixtures in process are needed for material and energy balances and for equipment design. A key factor in evaluating process simulation programs and design programs is the reliability of predicted thermophysical properties and phase equilibria. Such data are usually supplied as various forms of databases. DDB (Dortmund Data Bank) [1] and DIPPR (Design Institute for Physical Properties) [2] are well known such mixture and pure component physical properties database. It has been recognized that the absence of reliable data and correlation result in lack of confidence in design [3]. Several authors [3,4] have reviewed the effect of property estimation errors. For the past years, need for accurate data for comprehensive materials were not the serious problem. With the advances of process engineering, the need for thermophysical properties and calculation module is growing in Korea. Moreover, the growing demand for new material, and environmental and safety consideration, the industry demand for new data and models are rapidly increasing. With the financial support of MOCIE (Ministry of Commerce, Industry and Energy) in Korea, four universities (Korea University, Sogang University, Seoul National University and KAIST) collaborated to construct database and experimental services. The main purpose of KDB (Korea thermophysical Data Bank) project is to develop, organize and maintain useful data compilation and calculation programs. These data compilation must meet the need of industry in Korea.

2. Data Compilation

The database is composed of pure component property and mixture property database and their management system. Components are classified as hydrocarbon, polymers and

electrolytes.

2.1 Pure Component Properties

Entries to the pure component property databank are some 2000 hydrocarbons, 200 polymers and 2000 electrolytes. Fixed properties collected for each component are:

(Hydrocarbons)

Basic Properties:

Molecular Weight, Critical Data, Boiling Point, Freezing Point, Triple Point, Accentric Factor, Solubility Parameters, Heat of Combustion, Heat of Fusion, … etc

Molecular Properties:

Dipole Moment, Radius of Gyration, Van der Waals Volume/Area

Point Properties:

Liquid Density, Heat of Vaporization, Surface Tension Dielectric Constant, Refractive index at given Temperature

Hazardous and Environmental Properties:

Flash Point, Flammability Limit, Auto Ignition Temperature, NFPA Rating

(Polymers)

Glass Transition Temperature, Melting Point, Solubility Parameters, Dielectric Constants, Refractive Index, Surface Tension, … etc.

(Electrolytes)

Molecular Weights, Ionic Valence, Solid Density, Gibbs Free Energy, … etc

They are given with values in original units, references and accuracy information when possible. Raw experimental data for temperature dependent properties such as vapor pressure, heat capacities viscosity, thermal conductivity and surface tension are also

given with their regression coefficients.

2.2 Mixture Properties

About 5000 sets of phase equilibrium data and mixture properties are provided for hydrocarbons VLE, polymer solubility and electrolyte solubility. They are provided with references, accuracy information and experimental methods. Fig. 4 shows typical binary VLE input program interface.

- Vapor-Liquid Equilibrium Data Collection (4602 Sets)
- Polymer Finite Solubility (431 Sets)
- Polymer Infinite Solubility (222 Sets)
- Aqueous Electrolyte Solution Solubility (501 Sets)

2.3 Miscellaneous Data

Atomic weights, dimension conversion table, physical constants, property definition table and other miscellaneous data tables are also given for future uses.

2.4 Databank Management Program

Databank management program is composed of 4 parts - data input programs, data verification / regression programs, data transfer program and data search / view program. Working data are stored in local computers and verified data are stored in DBMS server using Microsoft SQL Server software. Fig.1 and Fig.3 shows typical data input program for hydrocarbon pure component data.

3. CALCULATION MODULES

Calculation modules include FORTRAN 77 source codes for physical property and phase equilibrium calculation. Simple process design programs were also included for the test of thermophysical property calculation modules. List of programs available for property calculations are as follows;

(Hydrocarbons)

- Vapor Pressure Calculation, Heat of Vaporization Calculation, Gas/Liquid Density Calculation, Gas/Liquid Viscosity Calculation, Gas/Liquid Thermal Conductivity Calculation, Gas/Liquid Heat Capacity Calculation
- Vapor-Liquid Equilibrium Calculation

(Polymers)

- Density Estimation , Glass Transition Temperature Estimation ,Heat Capacity Estimation , Heat of Fusion Estimation, Cohesive Energy Estimation ,Refractive Index Estimation ,Solubility Parameter Estimation,
- Polymer Solubility Calculation

(Aqueous Electrolyte Solutions)

- Freezing Point Lowering Calculation, Solubility Calculation ,Solution Density Calculation , Solution Viscosity Calculation, Solution Vapor Pressure Calculation ,
- Vapor-Liquid Equilibrium Calculation

Essentially, all the property calculation modules for polymer properties are based on group-contribution methods. Models used for equilibrium calculations are as follows;

(Hydrocarbons VLE)

- Equation of States : SRK EOS (with Wong-Sandler Mixing Rule) ,PR EOS (with Wong-Sandler Mixing Rule) , Nonrandom Lattice Fluid Model
- Activity Models : WILSON Model ,UNIQUAC Model , UNIFAC Model

(Polymer Solutions)

- High-Danner Model, UNIFAC-Free Volume Model, Nonrandom Lattice Fluid Model

(Aqueous Electrolyte Solutions)

- Pitzer Model, Chen Model, Bromley Model, Meissner Model, UNIQUAC Model

4. EXPEIMENTAL CAPABILITIES

Besides the effort to collect data in the literature, four universities in Korea collaborated to enhance their experimental capabilities in their specialized fields. Data producing projects were performed in accordance with local industry's demand on specific data.

5. WEB SERVICE

Complied physical property data and coefficients for calculation modules can be accessed using Internet WEB site. (http://thermo.korea.ac.kr) WEB service includes following interface to the databank.

- Unit Conversion
- Atomic Weights
- Pure Component Fixed Properties
- Temperature Dependent Pure Properties
- Binary VLE Databank
- Polymer Solubility Databank
- Aqueous Electrolyte Solution Databank

Typical database search result is shown in Fig.2.

6. PROSPECT

After three years of developing the basic structure and collecting literature data under the MOCIE's support, still the more effort have to be continued to meet the need of academy and industry. Furthermore, it is estimated that 40-60 % of the budget of a long-term software is spent on maintenance. With the aid of KIChE (Korea Information Center for Chemical Engineering), the databank is still growing and refining its

contents.

7. CONCLUSIONS

Current status of the database project in Korea was briefly summarized. The project is intended to gather data on specialized fields and construct database, enhance experimental capability and produce data, and develop computational modules for thermophysical properties and equilibria.

ACKNOWLEGMENT

The authors are grateful to the MOCIE and KIChE for the financial support.

REFERENCES

1. Gmehling, J., Onken, U. and Arlt, W., "Vapor-Liquid Equilibrium Data Collection", DECHEMA, Frankfurt (1978)
2. Daubert, T.E. and Danner, R. P., "Data Compilation, Tables of Properties of Pure Compouds", DIPPR, New York (1985)
3. Larsen, A.H., "Data Quality for Process Design", *Fluid Phase Equilibria*, **29**, 47 (1986)
4. Squrires, E.W. and Orchard, J.C., "How Gas-plant Performance Compares with Process Design", *Oil and Gas J.* , **66**, 36 (1968)
5. William, C.C. and Albright, M.A., "Better Data Saves Energy", *Hydrocarbon Proc.*, May, 115 (1976)
6. Zudkevitch, D. "Design-data importance of accuracy", Encyclopedia of Chemical Processing and Design, Mecketta, J. ed., **14**, 431, (1981)

FIGURE CAPTIONS

Fig. 1. Typical Data Input Program of KDB

Fig. 2. Internet Search Result of binary VLE Data

Fig. 3. Pure Component Experimental Data Input Program of KDB

Fig. 4. Binary VLE Experimental Data Input Program of KDB

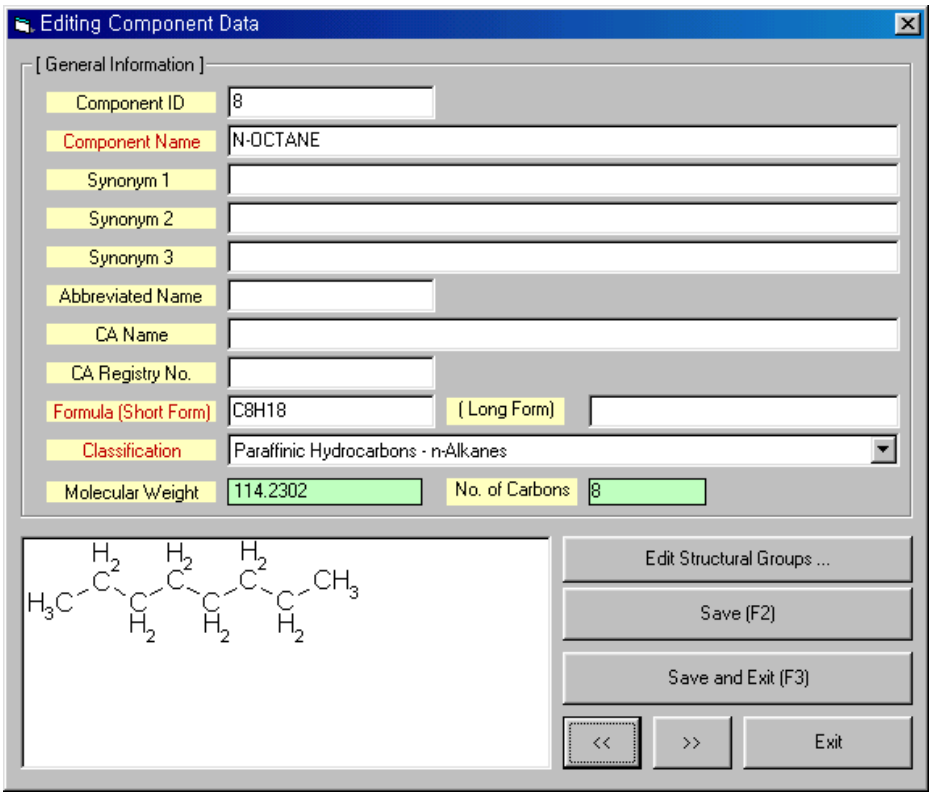

Fig. 1. Typical Data Input Program of KDB

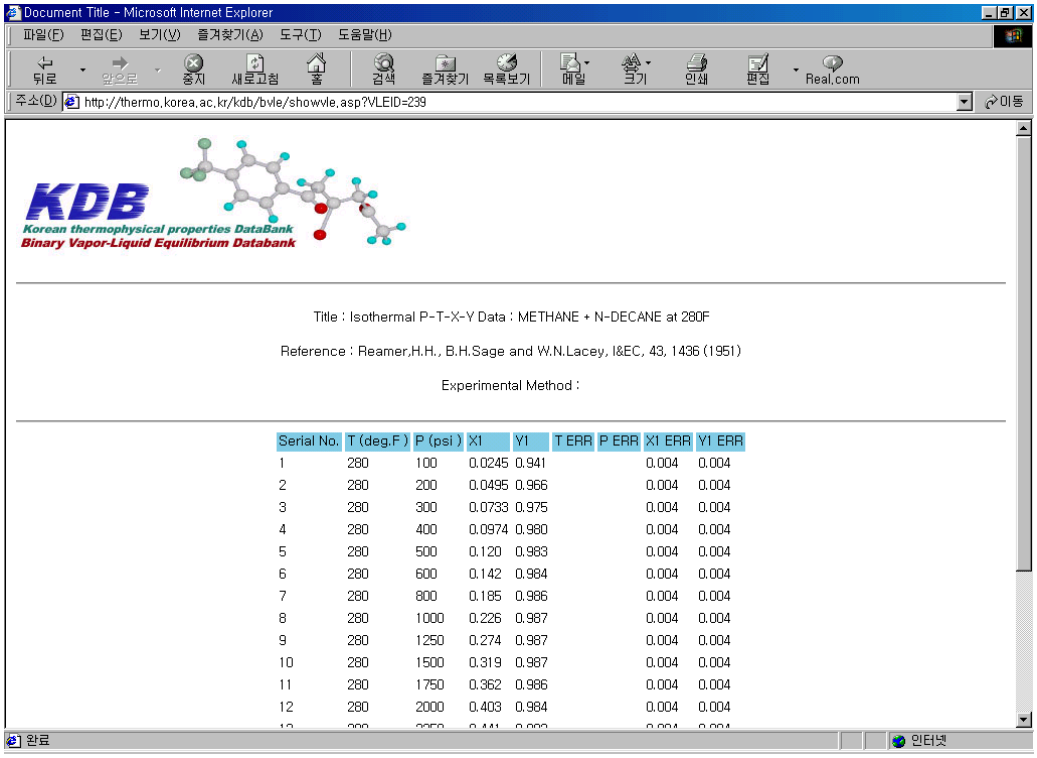

Fig. 2. Internet Search Result of binary VLE Data

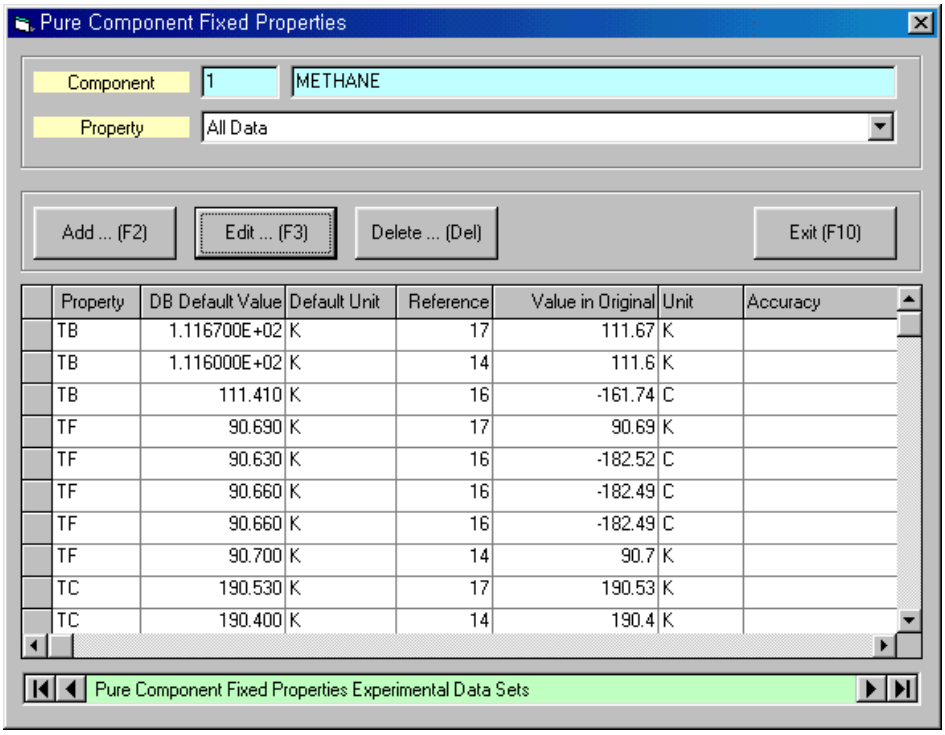

Fig. 3. Pure Component Experimental Data Input Program of KDB

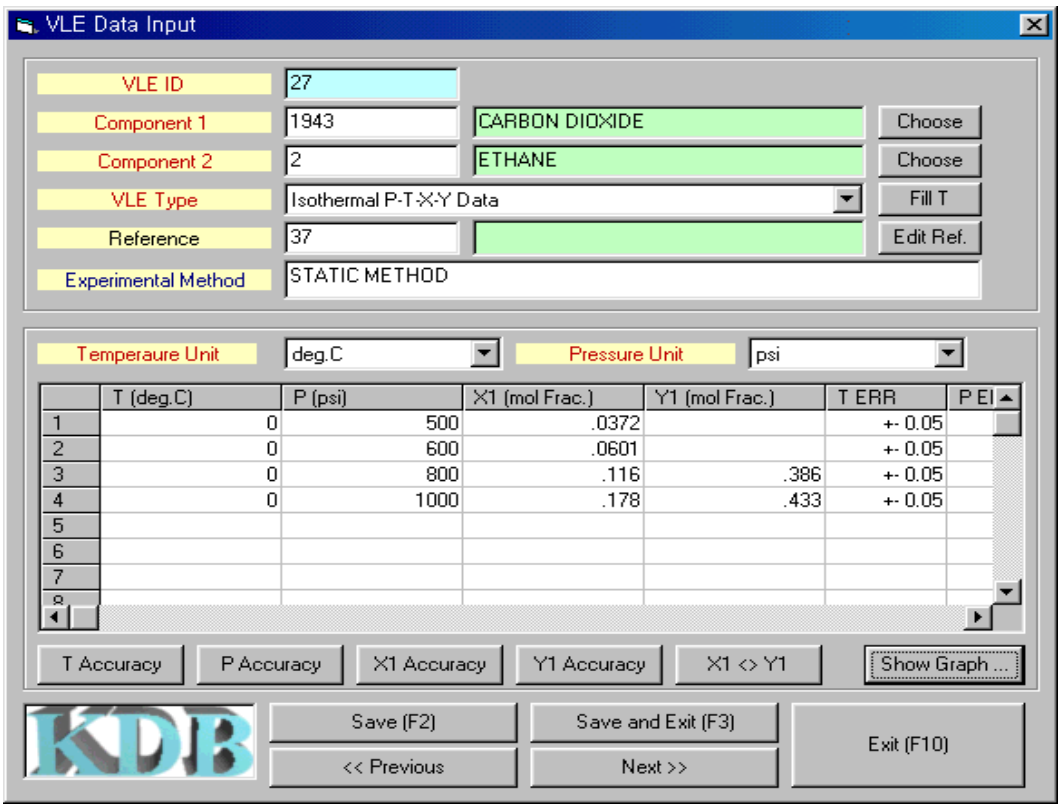

Fig 4. Binary VLE Experimental Data Input Program of KDB